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Charge transfer phenomena in carbon nanotube heterodevices

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Abstract. We describe the transfer of electric charge in junctions between a metal and carbon nanotube as well as between metallic and semiconducting carbon nanotubes. The long range Coulomb interaction drastically modifies the charge transfer phenomena in one-dimensional nanotube systems compared to conventional semiconductor heterostructures. Being brought into a contact with a metal, conducting nanotube accumulates electric charge whose density decays slowly with the distance from the junction. The length of the Schottky barrier in nanotube heterojunctions varies from the distances of the order of the nanotube radius (nanometers) to the distances of the order of the nanotube length (microns) depending on a doping strength. The Schottky barrier height shows pronounced asymmetry under the forward and reverse bias. This results in rectifying behavior of heterojunctions, in agreement with recent experimental observations by Z. Yao *et al.* and M. Fuhrer *et al.*

Introduction

Physical properties of single-wall carbon nanotubes (SWNTs) are determined by their geometry [1]. Depending on the wrapping vector, SWNTs can be either metallic or semiconducting with the energy gap in sub-electronvolt range [2, 3]. Strong Coulomb interaction in 1D SWNTs results in a variety of correlation phenomena. Away from half-filling the correlations are well described by the Luttinger liquid-like model. In particular, the non-Fermi liquid ground state of the system results in a power-law suppression of the density of electronic states near the Fermi level. This was observed in single- [4] and, presumably, multi-wall [5] nanotubes, as well as in junctions between metallic SWNTs [6].

Of particular interest are carbon nanotube devices. The simplest can be fabricated by contacting two nanotubes with different conducting properties. Electron transport in such nanotube heterojunctions has been investigated in two recent experiments. Yao *et al.* have treated heterojunctions at the kinks in SWNTs [6] whereas McEuen *et al.* have explored contacts of crossed nanotubes [7]. Both groups have reported asymmetry in the $I-V$ characteristics of heterojunctions (rectifying behavior). This might be surprising, since one expects no charge transfer in contacts between two isolated SWNTs made of the same material.

In this work we study charge transfer phenomena in nanotube heterojunctions taking true long-range Coulomb interaction into account. We concentrate on junctions between a metal and a nanotube and between metallic and semiconducting SWNTs. Their equilibrium and non-equilibrium characteristics are analysed by solving the Poisson equation self-consistently.

1. Method

Consider metallic or semiconducting SWNT with the axis z . We assume that conducting p_z electrons in SWNT are confined to the surface of a cylinder of radius R . SWNT is

surrounded by coaxial cylindrical metallic gate of radius $R_s \gg R$. The Poisson equation relates the potential $\varphi(z)$ at the surface of SWNT to 1D charge density $\rho(z)$ in SWNT and the potential $\Phi(z)$ of the gate,

$$\varphi_q = \varphi_q^{(\rho)} + \varphi_q^{(g)}, \quad \varphi_q^{(\rho)} = U_q \rho_q, \quad \varphi_q^{(g)} = M_q \Phi_q, \quad (1)$$

with

$$U_q = \frac{2}{\kappa} \left\{ I_0(qR) K_0(qR) - I_0^2(qR) \frac{K_0(qR_s)}{I_0(qR_s)} \right\}, \quad (2)$$

$$M_q = \frac{I_0(qR)}{I_0(qR_s)}. \quad (3)$$

Here κ is the dielectric constant of the media and I_0, K_0 are the modified Bessel functions. The kernel (2) describes the long-range Coulomb interaction, $U(x) = 1/\kappa|z|$, for $R \ll |z| \ll R_s$. The interaction is screened at large distances $|z| \gg R_s$, so that $U(q=0) = 1/C = (2/\kappa) \ln(R_s/R)$, C being the capacitance of SWNT per unit length.

In equilibrium, the charge density is related to the energy $\bar{E}_0(z) = E_0(z) - E_F$ of the gapless point (charge neutrality level) of graphite E_0 counted from the Fermi level E_F . At zero temperature we obtain [8],

$$\rho(z) = e \int_0^{\bar{E}_0(z)} dE \nu(E), \quad (4)$$

with the density of electronic states ν and $e > 0$. Equation (4) is valid if $\bar{E}_0(z)$ varies slowly on the scale of the Fermi wavelength.

We restrict our consideration to low energies $|\bar{E}_0(z)| < \Delta^{(1)}$ and neglect the effect of higher 1D subbands $(\Delta^{(1)}/(\hbar v_F/R)) = 1, 2/3$ for metallic/semiconducting SWNT). The densities of states in metallic and semiconducting SWNTs are given by,

$$\nu_M = \frac{4}{\pi \hbar v_F}, \quad \nu_S = \frac{4}{\pi \hbar v_F} \frac{|E| \Theta(|E| - \Delta)}{\sqrt{E^2 - \Delta^2}}, \quad (5)$$

$\Delta = \hbar v_F/3R$ being the half energy gap in semiconducting SWNT, and $v_F \simeq 8.1 \times 10^5$ m/s being the Fermi velocity.

In turn, the charge neutrality level is related to the electrostatic potential (1),

$$\bar{E}_0(z) + e\varphi(z) = \text{const.} \quad (6)$$

In what follows we will solve Eqs. (1), (4), (6) self-consistently for two situations.

2. Metal-nanotube contacts

We consider first metallic SWNT ($z > 0$) contacting the xy -plane of a metallic electrode ($z < 0$) at $z = 0$ (Fig. 1(a)). The potential of the xy -plane is chosen to be zero, and the potential of the gate is V_g . Assuming the metal electrode to be a perfect conductor we neglect the band bending in it. The charge neutrality point in SWNT at $z \rightarrow +0$ is shifted from the Fermi level by an amount $\bar{E}_0(+0) = \Delta W$ equal to the difference $\Delta W = W_M - W_{NT}$ of the work functions of the electrode and SWNT, so that $\text{const} = \Delta W$ in Eq. (6).

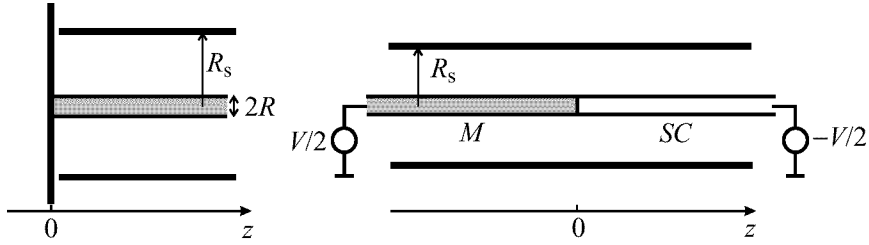


Fig. 1. Two systems under consideration: SWNT contacted to a metal (a) and heterojunction between metallic (M) and semiconducting (SC) nanotubes (b). The potential V_g is applied to the gate electrode.

In order to fulfil the boundary condition $\varphi(r, z = 0) = 0$ for the potential in xy -plane we solve Eqs. (1), (4), (6) with antisymmetric sources. The solution for the charge density has the form,

$$\rho_q = -\frac{2iq}{q^2 + \alpha^2} \frac{(\Delta W/e - M_q V_g)}{U_q + 1/(e^2 v_M)}, \quad (7)$$

with $\alpha \rightarrow 0$.

To evaluate the solution in the intermediate distance range $R \ll z \ll R_s$ we use the asymptotic $U_q = -(2/\kappa) \ln(qR)$. The deviation of the charge neutrality point from the Fermi level is given by,

$$\bar{E}_0(z) = \frac{\Delta W}{g} \frac{1}{\ln(z/R)} - \frac{ceV_g}{g} \frac{z}{R_s \ln(R_s/R)}, \quad (8)$$

where $c = (1/\pi) \int dx |I_0(x)|^{-1} \simeq 1.33$ and the Coulomb interaction $g = 2e^2 v_M / \kappa$ is supposed to be strong, $g \gg 1$. One can infer the interaction parameter $g \simeq 5$ from the experimental data [4, 6].

Using the asymptotics $U_q = (2/\kappa) \ln(R_s/R)$, and $M_q = 1$ for $|q| \ll R_s^{-1}$ we obtain the result at large distances $z \gg R_s$,

$$\bar{E}_0 = \frac{\Delta W - eV_g}{1 + g \ln(R_s/R)}. \quad (9)$$

In this regime the electric field of the electrode at $z = 0$ is well screened by the gate and the charge density in SWNT can be effectively controlled by the gate voltage.

3. All-nanotube heterojunctions

We will consider the heterojunction joining metallic ($z < 0$) and semiconducting ($z > 0$) SWNTs at the angle π (Fig. 1b) and perform its modeling using the formalism of Section 1. Since experimental values [6, 7] of the heterojunction conductance are typically small, $G/(e^2/h) \sim 10^{-3} - 10^{-2}$, we will assume low transparency $T \ll 1$ of the barrier at the interface between the nanotubes. In this case the electrons in SWNTs are described by the equilibrium Fermi distribution, even if the voltage V is applied to the junction. Assuming that the electrodes are connected to SWNTs at large distances $d \gg R_s$ from the junction we obtain $\varphi^{(g)}(z) = V_g$. This allows us to rewrite Eq. (6) as follows,

$$\bar{E}_0(z) + e\varphi^{(\rho)}(z) = \mu \pm eV/2, \quad (10)$$

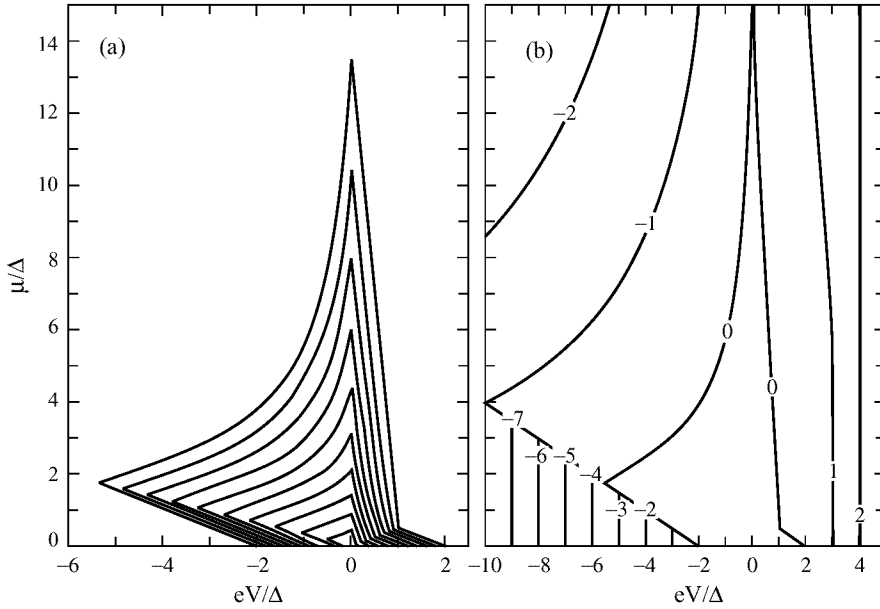


Fig. 2. The height u of the Schottky barrier (a) and the current I through the heterojunction (b) at zero temperature as functions of the electro-chemical potential μ and bias voltage V . The contour lines (a) correspond to $u/\Delta = 0, 0.1, \dots, 0.9$ from periphery to origin. The energies μ, eV are in units of Δ . The current is in units of $2e\Delta T_i/(\pi\hbar)$.

where $\mu \pm eV/2$ are the electro-chemical potentials for holes in metallic and semiconducting SWNTs and $\mu = \Delta W - eV_g$. Note that the problem becomes non-linear due to the presence of semiconducting SWNT.

Figure 2(a) shows the result for the SB height u defined as the minimum energy of electron or hole excitation required to transfer the elementary charge across the junction in the absence of tunneling through the SB. The SB height shows pronounced asymmetry as a function of the bias voltage. At small electrochemical potential the SB height at forward (reverse) bias is determined by the energy of the valence (conduction) band in the "bulk" of semiconducting SWNT, $x \rightarrow \infty$, with respect to the Fermi level, $u_{f(r)}^{(b)} = \Delta \mp \tilde{E}_0(\infty)$, with $\tilde{E}_0(\infty) = \mu + eV/2$. This corresponds to straight portions of contour lines in the lower part of Fig. 2 (a). In particular, the positive V_+ and negative V_- threshold voltages at which the SB vanishes ($u_{f(r)}^{(b)} = 0$) are given by $eV_{\pm}^{(b)} = \pm 2\Delta - 2\mu$.

Straight portions of contour lines (Fig. 2(a)) are interrupted by cusps. At forward bias the cusps occur along the line $eV = 2\mu$ (Fig. 2(a)) where the charge density in metallic SWNT and the band bending change sign. Above the point of a cusp, the height of a SB at forward (reverse) bias corresponds to the energy of the valence band at the interface of SWNTs, $x = 0$, counted from the Fermi level of semiconducting (metallic) nanotube, $u_{f(r)}^{(i)} = \Delta - \tilde{E}_0(\pm 0)$. The threshold voltages $V_{+(-)}^{(i)}$, correspond to suppression of a SB at the interface, $u_{f(r)}^{(i)} = 0$. Note that at $\mu \sim \Delta/2$ the positive threshold $eV_+^{(i)} \simeq \Delta$ is relatively insensitive to the electro-chemical potential, Fig. 2(a). This can be used for a rough estimate of the gap from experimental data.

The asymmetry of the $I - V$ characteristics and threshold voltages has been discovered

in recent experiments [6, 7]. According to the data of Ref. [6], both the thresholds V_+ , V_- shift upwards with the gate voltage. Moreover, the positive threshold shifts less than the negative one. Such behavior is consistent with our model in the regime of moderate doping, $0.5 < \mu/\Delta < 1.8$ (Fig. 2). However, the blockade region of 3–4 V detected in the experiment is somewhat wider than the theoretical estimate, $V_+ - V_- < 6.5\Delta \simeq 2$ eV. The extra voltage drop could be due to potential disorder in semiconducting SWNT [9] and/or an additional SB at the interface between semiconducting SWNT and metallic electrode.

We now check the model against the experimental data of Ref. [7]. The measured width of the blockade region, 0.5–0.7 V, agrees with the theoretical estimate. The gap in semiconducting SWNT, $\Delta \simeq eV_+$, evaluates at $\Delta = 0.19, 0.29$ eV for the two devices studied [7]. These values are in the expected range $\Delta \sim 0.25\text{--}0.35$ eV [2, 3]. A smooth onset of the current over the range $\sim 0.1\text{--}0.3$ eV around threshold voltages is naturally associated with quantum tunneling through a “leaky” SB (thermal energies are much smaller, $k_B T \simeq 5$ meV). Finally, the step-like feature of the current under reverse bias almost certainly corresponds to the reconstruction of the band profile due to the Fermi level entering the conduction band of semiconducting SWNT.

4. Conclusions

To conclude, we have studied the electronic properties of carbon nanotube heterojunctions and provided explanation for the main features of recent experimental data [6, 7]. Due to the long-range Coulomb interaction, the charge transfer phenomena in one-dimensional nanotube systems differs drastically from those in conventional semiconductor heterostructures. This creates new challenges in the design of novel electronic devices.

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